



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 PM UTC

PDB ID : 1NDB / pdb_00001ndb
Title : Crystal structure of Carnitine Acetyltransferase
Authors : Jogl, G.; Tong, L.
Deposited on : 2002-12-09
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

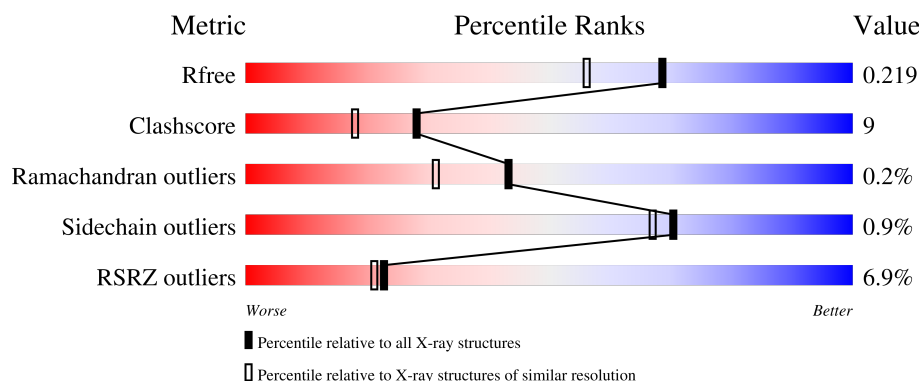
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	596	5% 81% 18% .
1	B	596	8% 78% 21% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	Se	0	0	0
			4757	3034	820	875	8	20			
1	B	596	Total	C	N	O	S	Se	0	0	0
			4757	3034	820	875	8	20			

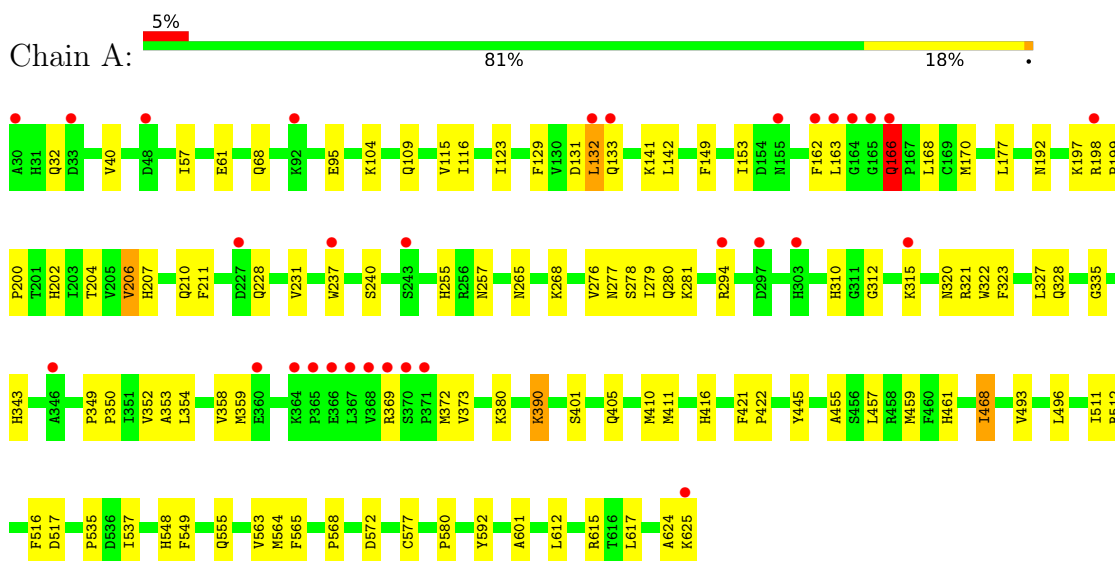
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	584	Total	O	0	0
			584	584		
2	B	462	Total	O	0	0
			462	462		

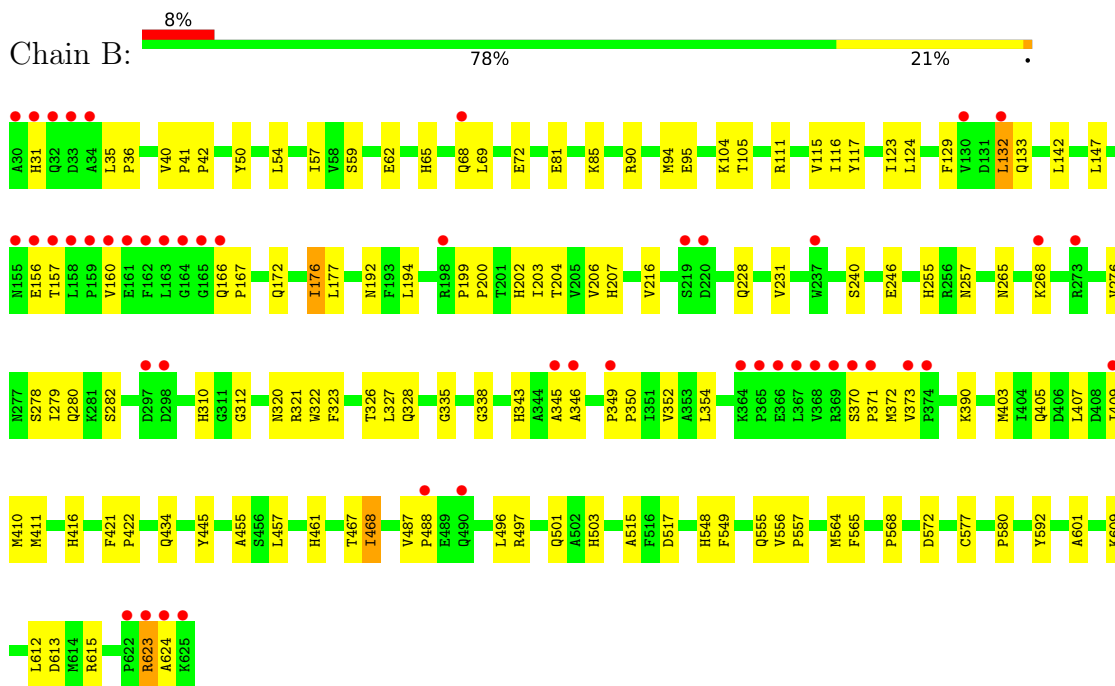
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Carnitine Acetyltransferase



• Molecule 1: Carnitine Acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.88Å 89.65Å 119.44Å 90.00° 127.46° 90.00°	Depositor
Resolution (Å)	29.69 – 1.80 29.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.69-1.80) 97.5 (29.69-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.219 0.192 , 0.219	Depositor DCC
R_{free} test set	17177 reflections (7.15%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10560	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/4852	0.86	11/6540 (0.2%)
1	B	0.33	0/4852	0.85	15/6540 (0.2%)
All	All	0.35	0/9704	0.85	26/13080 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ILE	N-CA-C	7.93	119.73	112.43
1	B	176	ILE	N-CA-C	7.44	119.47	111.58
1	A	343	HIS	N-CA-C	7.03	121.12	112.54
1	A	166	GLN	CA-C-N	6.73	126.70	119.76
1	A	166	GLN	C-N-CA	6.73	126.70	119.76
1	B	343	HIS	N-CA-C	6.54	120.51	112.54
1	A	549	PHE	N-CA-C	6.12	118.76	108.23
1	B	517	ASP	N-CA-C	6.06	117.55	111.07
1	A	517	ASP	N-CA-C	5.96	117.45	111.07
1	A	57	ILE	N-CA-C	5.83	118.76	113.10
1	A	445	TYR	N-CA-C	5.67	120.36	113.38
1	B	515	ALA	N-CA-C	-5.59	103.25	110.19
1	B	549	PHE	N-CA-C	5.57	117.81	108.23
1	B	345	ALA	N-CA-C	5.50	117.08	111.14
1	B	203	ILE	N-CA-C	-5.48	101.18	108.96
1	B	323	PHE	N-CA-C	5.40	119.35	112.87
1	B	468	ILE	N-CA-C	-5.37	100.68	108.36
1	B	467	THR	N-CA-C	5.26	117.82	109.24
1	A	40	VAL	N-CA-C	-5.23	102.00	107.60
1	B	346	ALA	N-CA-C	5.20	115.00	108.45
1	A	323	PHE	N-CA-C	5.20	119.11	112.87
1	A	468	ILE	N-CA-C	-5.19	100.94	108.36
1	A	353	ALA	N-CA-C	-5.18	105.71	111.36
1	B	40	VAL	N-CA-C	-5.18	102.06	107.60
1	B	445	TYR	N-CA-C	5.11	119.66	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	111	ARG	N-CA-C	5.04	119.41	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4733	88	0
1	B	4757	0	4733	80	0
2	A	584	0	0	12	0
2	B	462	0	0	6	0
All	All	10560	0	9466	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:MSE:HG2	1:A:373:VAL:H	1.31	0.95
1:A:132:LEU:HD22	1:A:132:LEU:H	1.39	0.87
1:A:624:ALA:O	1:A:625:LYS:HB2	1.76	0.86
1:B:623:ARG:HB3	1:B:623:ARG:NH1	1.90	0.85
1:A:32:GLN:HE22	1:A:170:MSE:H	1.28	0.81
1:B:265:ASN:HA	1:B:268:LYS:HE3	1.64	0.80
1:B:310:HIS:HD2	1:B:312:GLY:H	1.30	0.79
1:A:277:ASN:HD21	1:A:281:LYS:HE3	1.48	0.77
1:A:310:HIS:HD2	1:A:312:GLY:H	1.30	0.77
1:A:163:LEU:HB2	1:A:166:GLN:HG3	1.68	0.76
1:A:372:MSE:HG2	1:A:373:VAL:N	2.01	0.76
1:A:535:PRO:HB2	2:A:990:HOH:O	1.86	0.76
1:B:623:ARG:HB3	1:B:623:ARG:HH11	1.51	0.74
1:A:315:LYS:HG2	2:A:824:HOH:O	1.89	0.72
1:B:370:SER:HB2	1:B:371:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:CD2	1:A:312:GLY:H	2.12	0.68
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.76	0.67
1:A:459:MSE:HE3	1:A:511:ILE:HG22	1.75	0.67
1:A:255:HIS:HD2	1:A:257:ASN:H	1.41	0.67
1:A:537:ILE:HG22	2:A:990:HOH:O	1.94	0.66
1:B:117:TYR:CE1	1:B:403:MSE:HE3	2.30	0.66
1:B:132:LEU:HD12	1:B:133:GLN:H	1.60	0.66
1:B:310:HIS:CD2	1:B:312:GLY:H	2.12	0.66
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.78	0.66
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.32	0.65
1:A:322:TRP:H	1:A:328:GLN:NE2	1.96	0.64
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.33	0.64
1:A:277:ASN:ND2	1:A:281:LYS:HE3	2.12	0.64
1:A:255:HIS:CD2	1:A:257:ASN:H	2.15	0.63
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.64	0.63
1:A:132:LEU:H	1:A:132:LEU:CD2	2.12	0.61
1:A:358:VAL:HG12	1:A:359:MSE:HE2	1.82	0.61
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.82	0.61
1:A:354:LEU:C	1:A:354:LEU:HD23	2.27	0.59
1:A:132:LEU:HD22	1:A:132:LEU:N	2.16	0.59
1:B:497:ARG:O	1:B:501:GLN:HG2	2.03	0.59
1:B:95:GLU:OE1	1:B:461:HIS:HE1	1.86	0.59
1:A:322:TRP:H	1:A:328:GLN:HE22	1.51	0.58
1:B:104:LYS:HG3	1:B:105:THR:N	2.19	0.58
1:B:246:GLU:OE2	1:B:390:LYS:HE2	2.03	0.58
1:B:555:GLN:HE21	1:B:580:PRO:HG2	1.69	0.57
1:A:163:LEU:CB	1:A:166:GLN:HG3	2.34	0.57
1:A:555:GLN:HE21	1:A:580:PRO:HG2	1.69	0.57
1:B:354:LEU:C	1:B:354:LEU:HD23	2.30	0.56
1:B:276:VAL:O	1:B:280:GLN:HG3	2.04	0.56
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.87	0.55
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.88	0.55
1:A:162:PHE:O	1:A:163:LEU:HD22	2.06	0.55
1:A:410:MSE:HG2	1:A:601:ALA:HA	1.88	0.55
1:B:457:LEU:HG	2:B:767:HOH:O	2.07	0.55
1:A:32:GLN:NE2	1:A:170:MSE:H	2.01	0.54
1:B:496:LEU:C	1:B:496:LEU:HD23	2.33	0.54
1:B:322:TRP:H	1:B:328:GLN:NE2	2.05	0.54
1:B:81:GLU:HG3	2:B:688:HOH:O	2.07	0.54
1:A:537:ILE:CG2	2:A:990:HOH:O	2.54	0.54
1:A:197:LYS:HG2	2:A:935:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:HG2	2:B:914:HOH:O	2.08	0.53
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.43	0.53
1:B:407:LEU:HD21	1:B:409:ILE:HD11	1.88	0.53
1:A:410:MSE:HE3	1:A:411:MSE:O	2.09	0.53
1:B:59:SER:OG	1:B:62:GLU:HG3	2.09	0.52
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.91	0.52
1:A:123:ILE:HD12	1:A:411:MSE:HE2	1.92	0.52
1:B:410:MSE:HE3	1:B:411:MSE:O	2.09	0.52
1:B:132:LEU:CD1	1:B:133:GLN:H	2.23	0.52
1:A:207:HIS:HD2	1:A:240:SER:OG	1.93	0.51
1:A:104:LYS:HG2	1:A:109:GLN:CD	2.35	0.51
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.46	0.51
1:B:623:ARG:HH11	1:B:623:ARG:CB	2.22	0.51
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.45	0.51
1:A:163:LEU:CD2	1:A:168:LEU:HD11	2.40	0.51
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.45	0.51
1:B:555:GLN:HG2	1:B:557:PRO:HD3	1.92	0.51
1:A:276:VAL:O	1:A:280:GLN:HG3	2.10	0.50
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.46	0.50
1:A:496:LEU:C	1:A:496:LEU:HD23	2.37	0.50
1:A:142:LEU:C	1:A:142:LEU:HD23	2.37	0.50
1:A:132:LEU:HD12	1:A:237:TRP:CZ2	2.47	0.49
1:B:81:GLU:O	1:B:85:LYS:HG2	2.12	0.49
1:B:116:ILE:HD12	1:B:403:MSE:HE2	1.93	0.49
1:B:320:ASN:C	1:B:321:ARG:HG2	2.36	0.49
1:A:163:LEU:HD23	1:A:168:LEU:HD11	1.95	0.49
1:A:231:VAL:HG21	1:A:372:MSE:HE1	1.93	0.49
1:B:202:HIS:HD2	2:B:666:HOH:O	1.95	0.49
1:B:142:LEU:C	1:B:142:LEU:HD23	2.38	0.49
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.48	0.48
1:A:123:ILE:HG13	1:A:565:PHE:CZ	2.48	0.48
1:A:204:THR:HG21	1:A:279:ILE:HA	1.94	0.48
1:A:457:LEU:HG	2:A:720:HOH:O	2.13	0.48
1:A:192:ASN:C	1:A:192:ASN:HD22	2.21	0.48
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.95	0.48
1:B:123:ILE:HD12	1:B:411:MSE:HE2	1.96	0.48
1:B:231:VAL:HG21	1:B:372:MSE:SE	2.62	0.48
1:B:255:HIS:HD2	1:B:257:ASN:HB2	1.78	0.48
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.78	0.48
1:B:322:TRP:H	1:B:328:GLN:HE22	1.60	0.48
1:A:123:ILE:HG13	1:A:565:PHE:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.95	0.48
1:A:131:ASP:OD1	1:A:133:GLN:HG3	2.14	0.48
1:B:410:MSE:HG2	1:B:601:ALA:HA	1.96	0.47
1:B:204:THR:HG21	1:B:279:ILE:HA	1.96	0.47
1:A:265:ASN:HA	1:A:268:LYS:HE3	1.96	0.47
1:A:228:GLN:HG2	1:A:372:MSE:HG3	1.96	0.47
1:B:192:ASN:HD22	1:B:192:ASN:C	2.22	0.47
1:B:352:VAL:HG11	1:B:556:VAL:HG12	1.96	0.47
1:A:198:ARG:O	1:A:198:ARG:HG3	2.15	0.47
1:A:210:GLN:HE21	1:A:380:LYS:NZ	2.13	0.47
1:A:401:SER:O	1:A:405:GLN:HG3	2.15	0.47
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.96	0.47
1:B:177:LEU:HD23	1:B:327:LEU:HD12	1.97	0.47
1:A:411:MSE:CE	1:A:563:VAL:HG11	2.45	0.46
1:A:320:ASN:C	1:A:321:ARG:HG2	2.40	0.46
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.98	0.46
1:A:141:LYS:HZ1	1:A:369:ARG:NH2	2.13	0.46
1:A:390:LYS:HB3	1:A:390:LYS:NZ	2.31	0.46
1:A:535:PRO:C	2:A:990:HOH:O	2.59	0.46
1:B:31:HIS:CE1	1:B:167:PRO:HB3	2.51	0.46
1:A:68:GLN:NE2	2:A:1063:HOH:O	2.49	0.46
1:B:255:HIS:HE1	2:B:842:HOH:O	1.99	0.46
1:B:609:LYS:HE2	1:B:613:ASP:OD1	2.15	0.46
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.99	0.45
1:A:405:GLN:HG3	2:A:953:HOH:O	2.15	0.45
1:B:202:HIS:HE1	1:B:278:SER:O	1.98	0.45
1:B:207:HIS:HD2	1:B:240:SER:OG	1.99	0.45
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.98	0.45
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.28	0.45
1:B:310:HIS:HE1	2:B:948:HOH:O	2.00	0.45
1:B:564:MSE:HB3	1:B:577:CYS:SG	2.57	0.45
1:A:255:HIS:CD2	1:A:257:ASN:HB2	2.51	0.45
1:A:310:HIS:HE1	2:A:1026:HOH:O	2.00	0.45
1:B:228:GLN:CG	1:B:372:MSE:HE2	2.47	0.44
1:B:548:HIS:HE1	1:B:572:ASP:OD1	1.99	0.44
1:B:228:GLN:HG3	1:B:372:MSE:HE2	1.99	0.44
1:B:68:GLN:O	1:B:72:GLU:HG3	2.18	0.44
1:B:124:LEU:HG	1:B:338:GLY:HA2	2.00	0.44
1:A:237:TRP:HH2	2:A:835:HOH:O	2.00	0.44
1:B:372:MSE:CG	1:B:373:VAL:N	2.79	0.44
1:B:123:ILE:HG13	1:B:565:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HG23	1:B:282:SER:HB3	1.99	0.44
1:A:349:PRO:HA	1:A:352:VAL:HG22	2.00	0.43
1:A:109:GLN:NE2	2:A:992:HOH:O	2.51	0.43
1:A:228:GLN:CG	1:A:372:MSE:HG3	2.48	0.43
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.54	0.43
1:A:202:HIS:HE1	1:A:278:SER:O	2.02	0.42
1:B:31:HIS:CE1	1:B:160:VAL:HG11	2.54	0.42
1:B:199:PRO:HA	1:B:200:PRO:HD3	1.89	0.42
1:A:95:GLU:OE1	1:A:461:HIS:HE1	2.02	0.42
1:B:157:THR:HG22	1:B:157:THR:O	2.19	0.42
1:A:61:GLU:H	1:A:61:GLU:CD	2.26	0.42
1:B:176:ILE:HA	1:B:326:THR:HG21	2.01	0.42
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.35	0.42
1:B:65:HIS:CE1	1:B:69:LEU:HD11	2.54	0.42
1:A:564:MSE:HB3	1:A:577:CYS:SG	2.60	0.42
1:B:90:ARG:O	1:B:94:MSE:HG2	2.19	0.42
1:B:434:GLN:HG3	1:B:503:HIS:CE1	2.54	0.42
1:B:172:GLN:OE1	1:B:350:PRO:HG2	2.20	0.42
1:B:206:VAL:HG22	1:B:320:ASN:OD1	2.20	0.42
1:A:199:PRO:HA	1:A:200:PRO:HD3	1.92	0.41
1:A:206:VAL:HG22	1:A:211:PHE:CD2	2.55	0.41
1:B:41:PRO:HA	1:B:42:PRO:HD3	1.95	0.41
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.55	0.41
1:B:487:VAL:HA	1:B:488:PRO:HD3	1.88	0.41
1:B:147:LEU:HD11	1:B:216:VAL:HB	2.02	0.41
1:B:192:ASN:ND2	1:B:194:LEU:H	2.19	0.41
1:B:349:PRO:O	1:B:352:VAL:HG22	2.21	0.41
1:A:516:PHE:CD1	1:A:516:PHE:C	2.99	0.41
1:B:35:LEU:HA	1:B:36:PRO:HD3	1.95	0.40
1:A:149:PHE:CE1	1:A:153:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/596 (100%)	578 (97%)	16 (3%)	0	100	100
1	B	594/596 (100%)	578 (97%)	14 (2%)	2 (0%)	36	25
All	All	1188/1192 (100%)	1156 (97%)	30 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	624	ALA
1	B	623	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/504 (104%)	520 (99%)	4 (1%)	73	70
1	B	524/504 (104%)	519 (99%)	5 (1%)	68	64
All	All	1048/1008 (104%)	1039 (99%)	9 (1%)	70	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	166	GLN
1	A	206	VAL
1	A	390	LYS
1	B	132	LEU
1	B	156	GLU
1	B	166	GLN
1	B	405	GLN
1	B	615	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	65	HIS
1	A	68	GLN
1	A	84	GLN
1	A	109	GLN
1	A	112	GLN
1	A	133	GLN
1	A	135	GLN
1	A	155	ASN
1	A	187	GLN
1	A	192	ASN
1	A	207	HIS
1	A	210	GLN
1	A	228	GLN
1	A	242	GLN
1	A	255	HIS
1	A	277	ASN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	405	GLN
1	A	447	GLN
1	A	461	HIS
1	A	503	HIS
1	A	526	GLN
1	A	548	HIS
1	A	550	ASN
1	A	555	GLN
1	A	619	GLN
1	A	620	ASN
1	B	65	HIS
1	B	68	GLN
1	B	84	GLN
1	B	109	GLN
1	B	112	GLN
1	B	135	GLN
1	B	155	ASN
1	B	187	GLN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	228	GLN
1	B	255	HIS
1	B	264	ASN
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	447	GLN
1	B	461	HIS
1	B	491	GLN
1	B	501	GLN
1	B	503	HIS
1	B	526	GLN
1	B	548	HIS
1	B	555	GLN
1	B	605	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	576/596 (96%)	-0.03	31 (5%) 31 30	5, 12, 29, 71	0
1	B	576/596 (96%)	0.36	48 (8%) 17 15	8, 17, 41, 70	0
All	All	1152/1192 (96%)	0.16	79 (6%) 23 21	5, 14, 33, 71	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	9.4
1	A	164	GLY	9.1
1	A	165	GLY	7.9
1	A	371	PRO	7.7
1	B	368	VAL	6.9
1	B	163	LEU	6.6
1	A	367	LEU	6.5
1	A	163	LEU	6.4
1	B	624	ALA	6.3
1	B	162	PHE	5.6
1	B	373	VAL	5.5
1	B	625	LYS	5.5
1	A	162	PHE	5.5
1	B	34	ALA	5.4
1	A	625	LYS	5.4
1	A	166	GLN	5.4
1	A	369	ARG	5.3
1	B	367	LEU	5.3
1	A	132	LEU	4.9
1	B	157	THR	4.7
1	B	623	ARG	4.6
1	B	31	HIS	4.6
1	B	237	TRP	4.3
1	B	30	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	SER	4.3
1	B	622	PRO	4.2
1	B	371	PRO	4.2
1	B	165	GLY	4.0
1	B	156	GLU	4.0
1	B	132	LEU	3.8
1	B	160	VAL	3.8
1	B	155	ASN	3.8
1	B	33	ASP	3.7
1	B	370	SER	3.7
1	B	32	GLN	3.6
1	B	346	ALA	3.6
1	B	158	LEU	3.5
1	B	164	GLY	3.4
1	B	369	ARG	3.3
1	B	161	GLU	3.3
1	A	243	SER	3.1
1	B	159	PRO	3.1
1	B	219	SER	3.0
1	A	227	ASP	3.0
1	B	365	PRO	2.9
1	A	133	GLN	2.9
1	B	345	ALA	2.9
1	A	198	ARG	2.9
1	A	237	TRP	2.8
1	A	364	LYS	2.8
1	A	155	ASN	2.8
1	A	365	PRO	2.8
1	A	33	ASP	2.8
1	B	364	LYS	2.8
1	A	30	ALA	2.6
1	B	366	GLU	2.6
1	B	298	ASP	2.6
1	A	366	GLU	2.6
1	B	490	GLN	2.5
1	B	166	GLN	2.5
1	B	68	GLN	2.4
1	A	48	ASP	2.4
1	B	409	ILE	2.4
1	A	303	HIS	2.3
1	B	273	ARG	2.3
1	A	92	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	2.3
1	B	349	PRO	2.2
1	B	297	ASP	2.2
1	B	198	ARG	2.2
1	B	374	PRO	2.2
1	A	315	LYS	2.2
1	B	220	ASP	2.2
1	B	488	PRO	2.2
1	A	346	ALA	2.2
1	B	268	LYS	2.2
1	B	130	VAL	2.1
1	A	297	ASP	2.1
1	A	360	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.